Diethyl (3-carbethoxypropyl)phosphonate

Other names: Triethyl-4-phosphono butyrate
Butanoic acid, 4-(diethoxyphosphinyl)-, ethyl ester
Butyric acid, 4-diethylphosphono-, ethyl ester
Inchi: InChI=1S/C10H21O5P/c1-4-13-10(11)8-7-9-16(12,14-5-2)15-6-3/h4-9H2,1-3H3
InchiKey: FYESTJSRASJZOY-UHFFFAOYSA-N
Formula: C10H21O5P
SMILES: CCOC(=O)CCCP(=O)(OCC)OCC
Mol. weight [g/mol]: 252.25

Physical Properties

Property code	Value	Unit	Source
af	0.6865		Cheméo Relay (1.0)
gf	-553.22	kJ/mol	Cheméo Relay (1.0, beta)
hf	-1050.57	kJ/mol	Cheméo Relay (1.0)
hvap	78.25	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
log10ws	-0.59		Cheméo Relay (1.0)
logp	2.596		Crippen Method
mcvol	197.270	ml/mol	McGowan Method
pc	1927.03	kPa	Cheméo Relay (1.0, beta)
tb	579.19	K	Cheméo Relay (1.0)
tc	707.75	K	Cheméo Relay (1.0)
tf	231.57	K	Cheméo Relay (1.0)
vc	0.746	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2327697&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume